

FINAL REPORT

to the Office of Life Science Programs
National Aeronautics and Space Administration

INVESTIGATION OF THERMODYNAMIC MECHANISMS FOR THE PRODUCTION
OF COMPLEX COMPOUNDS ESSENTIAL FOR THE ORIGIN OF LIFE

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Oct. 1, 1964 to Sept. 30, 1965

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We have made a survey of the major compounds present in an ideal gas for all proportions of C, H, and O. Pressures of 10^{-3} to 300 atm were considered and temperatures of 300-1000°K. Results from the work were summarized in the paper, "Thermodynamic Equilibria in Prebiological Atmospheres" by M. O. Dayhoff, R. V. Eck, E. R. Lippincott, Science, Vol. 146, No. 3650, pp. 1461-1464, Dec. 11, 1964. The method has aroused considerable interest among astronomers for application to planetary and stellar atmospheres. Anders and his associates at Chicago have measured the compounds present in carbonaceous chondrite meteorites and found the molecular balance consistent with our computations in the asphalt region. French at Goddard Space Flight Center has pointed out that asphaltic compounds are also found in volcanic regions in carbonaceous igneous formations on earth (private communication).

A survey of the main compounds formed on addition of nitrogen and 1% of sulphur, phosphorus, chlorine and silicon has been made. The important results of this survey will be submitted for publication soon.

We considered the conditions under which certain biologically interesting compounds occurred in significant concentrations. A representative group of these was discussed in the paper cited above.

We have made a few preliminary estimates of the distribution of some compounds between the gas phase and an aqueous phase. Very little has been done to systematize the work in this field. Distribution constants between the gas and aqueous phase are scattered in the literature, if existent at all. We have found no published attempt to calculate free energies of solute molecules as a sum of contributions of groups of atoms. This is a necessary antecedent to a thermodynamic treatment of many organic compounds, comparable with our work in the gas phase.

We have made preliminary computations of steady-state systems which are at equilibrium except that the formation of certain compounds is forbidden. Thus, because of the very slow rate of certain reactions under some conditions, solid C, N₂ or possibly CO₂ or CO may be excluded from the reactants. These systems often simulate rather closely the products actually obtained in the laboratory experiments with electrical discharges or radiation in "primitive atmospheres."

We have considered simple living systems with a view to extrapolating backward to understand more primitive, extinct species. Two papers were delivered at the AAAS meeting in Montreal on this subject:

Surviving Relics of the Beginnings of Life
by Margaret O. Dayhoff

Ancestral Genetic Coding Mechanism: Surviving Evidences
by Richard V. Eck

Abstract of Papers Presented at the Montreal Meeting of the
American Association for the Advancement of Science, December 27, 1964

SURVIVING RELICS OF THE BEGINNINGS OF LIFE

Margaret O. Dayhoff

ANCESTRAL GENETIC CODING MECHANISM: SURVIVING EVIDENCES

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The organic evolution of living cells from non-living compounds was a complex process involving a sequence of systems of successively higher organization. These "metabolons" are no longer found living independently, but their nature can be deduced from the structure and function of the organelles, macromolecules, and chemicals of the living cells today, and from a knowledge of the nature of the evolutionary process and the knowledge of which structures are simple. Many of these necessary facts and processes are poorly understood today.

Simple Structures

In order to investigate what chemicals are "simple," a broad survey of the most stable mixtures of compounds formed from carbon, hydrogen, oxygen, nitrogen and sulfur was conducted. The concentrations of biologically interesting compounds in an ideal gas under all elemental compositions and plausible conditions of temperature and pressure was noted (Dayhoff, Lippincott, and Eck, Science, Dec. 11, 1964). These computations indicate that there were very few molecules of any complexity in an equilibrium primitive atmosphere. The probability of a whole reaction chain, such as those found in cells, coming together from such an extremely dilute mixture is exceedingly remote. Life must therefore have evolved starting as an organized functioning system of very simple compounds. The things available in major proportions are carbon dioxide, water, methane, hydrogen, carbon monoxide,

hydrogen sulfide, nitrogen, and possibly a "tar" phase of polyaromatic hydrocarbons. Ammonia is present in small concentration and organic compounds such as thiomethanol, acetic acid, formic acid, methanol and ethane are very dilute (about 10^{-10} mole percent). Such biologically interesting compounds as ribose and adenine would be so dilute that there would be only about a million molecules in the whole earth in a gaseous equilibrium.

These results lead us to search for some primordial aggregation of the simple compounds which could utilize radiant energy for metabolism.

Evolutionary Processes and Complex Structures

On the other hand, starting from the complexity of present living things, a number of inferences can be made about the structure of very early forms of life, by a mathematical analysis of the experimental results of the studies of the genetic code and of proteins. In spite of the billions of years that have passed, and the tremendous increase in complexity of organization of living chemistry that has occurred, there are still detectable (in the proportions and relationships of the components of nucleic acids and proteins) simple patterns which appear to be surviving traces of a very primitive mechanism from which the present extremely complex genetic mechanism must have evolved, step by step. The concept that the evolution of living things must have occurred one step at a time, and that every step must have been able to survive, becomes a very powerful approach to the unraveling of such patterns. If there were no such simple, general rule constraining the possible numbers of changes which could occur at each stage, it might seem impossible to find these still-living relics of the chemical organization of the very early forms of life.

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